Daily Kilometer-Scale MODIS Satellite Maps of $PM_{2.5}$ Describe Wintertime Episodes

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INTRODUCTION

The San Joaquin Valley (SJV) suffers from severe health-endangering episodes of $PM_{2.5}$ aerosol loadings in wintertime; episodes last approximately 5 days and differ in geographical distribution and composition. $PM_{2.5}$ stations are scattered; consequently the use of remote sensing to map variable regional patterns of these varying respirable aerosol concentrations is desirable. High-precision AOT retrievals can capture column particulate loading. However, $PM_{2.5}$mapping is challenging due to several reasons: particularly thin mixed layers (ML) and thus relatively low aerosol optical thickness (AOT) close to current measurement limits, variable and atypical composition of the aerosols, and complex surface bidirectional reflectance. However, the West does present some advantages in analysis. Air basins are isolated from long-distance transport, and experience predominant strong meteorological subsidence. Thus these Western basin regions have fewer problematic cases of overriding aerosol layers detached from the surface. To counter such local overriding, Chu et al.[1]have described an approach for the Eastern US, and He et al[2] have described a synoptic classification approach useful in Shanghai. The Bay Area Air Quality Management District (BAAQMD) expands our experience with the use of AOT, with lower $PM_{2.5}$ and several isolated sub-basins. We have prepared daily maps of episodes in each region. We present also a sequence of increasingly detailed statistical models, AOT initially appears to contribute little information; however, inclusion of weather information reveals its utility.

Lyapustin and Wang's MultiAngle Implementation of Atmospheric Correction (MAIAC) retrieval for AOT provided the most useful operational remote sensing information for these regions[3]. It provides high (1-km) spatial resolution maps and a high percentage of availability. Empirical regression methods have found that random effects regression models (aka mixed effects models, ME) employing AOT provide good estimates of ground $PM_{2.5}$ concentrations. Here, we attempt to extend these methods and evaluate the usefulness of AOT with greater physical analysis, based on DISCOVER-AQ[4] experience.

The definition of AOT, here written as τ_{Ext} is presented in Equation 1.

$$\tau_{ext} = \int_{z_{Sfc}}^{z_{Top}} \int_{0}^{r_{Max}} [\hat{\rho}_{aer} k_{ext}](RH) C_{StdCond}\, dr\, dz \qquad Eq. (1)$$

where, and $\hat{\rho}_{aer}$ is the distribution function of aerosol-particle mass density by radius. k_{ext} is the mass-based extinction coefficient, RH is relative humidity, and $C_{StdCond}$ allows unit conversion to μg m^{-3}, as integrated over all particle radius (*dr*) and all altitudes (*dz*) in a vertical column[5]. Equation 2. provides a simplification under the assumption that particles are contained within a mixed layer (ML) turbulently stirred to the height of the $PM_{2.5}$ monitor since mixing is often nearly complete after 11 AM on clear days[3,6].

$$\tau_{ext} = \int_{0}^{r_{Max}} \overline{[\hat{\rho}_{aer} k_{ext}](RH)} C_{StdCond}\, dr\, \Delta z_{mixed-layer} \qquad Eq. (2)$$

where $\Delta z_{mixed-layer}$ is the ML height and the indicated averaging is over the ML The RH effect for the ML, determined by conditions near the top where RH is highest. Particulate extinction must be negligible above the layer, as noted above.

However, the definition of $PM_{2.5}$ in μg m^{-3} is given by different integral of particle density,

$$\text{PM2.5} = \int_{0}^{r=1.25\,\mu\text{m}} \hat{\rho}_{\text{dry}}\, dr \qquad Eq. (3)$$

where, $\hat{\rho}_{\text{dry}}$ is the distribution function for dry aerosol-particle mass density integrated over particle radius, 0 to 1.25 μm (diameter 2.5). We assume that the relation between $\hat{\rho}_{\text{dry}}$ and $\hat{\rho}_{aer}$ (Eq. 1-2) corresponds to water evaporation. Due caution is required if measured dry density does not account for volatilization of organics, ammonia, and nitric acid. Note that the caveats and assumptions listed suggest many reasons why the ratio measured $PM_{2.5}$/ AOT *should be* quite variable. Similar caveats are given in many recent analyses[6]. Note, however, that these equations above do suggest that a consistent relationship between AOT and PM *might be* obtained for individual days in air basins with reasonably homogeneous particle characteristics and ML properties.

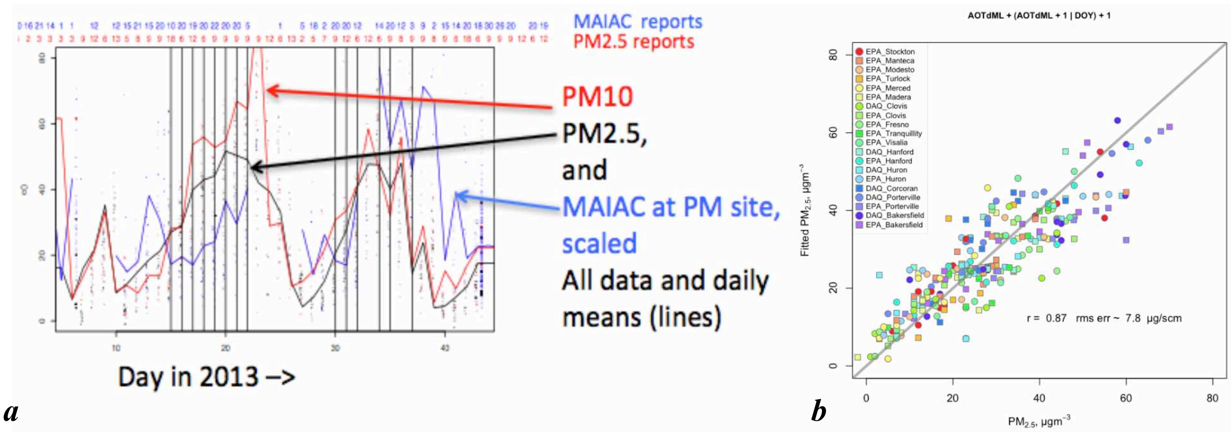
Our experience forecasting $PM_{2.5}$ for DISCOVER-AQ flights[4] in the San Joaquin Valley in 2013 emphasized that globally useful large scale models like GEOS and MERRA re-analyses do not capture composition nor represent ML depth accurately for these California regions. (Confirmed by A. Da Silva, personal communication, 2013, 2017). We found that the NOAA RAP (RAPid refresh product) constrains its ML depths based on available, recent, richly observed humidity and temperature and so captures ML well, at moderate spatial resolution, 14 km. These ML depths varied geographically but the vertical variation was similar from day to day. The combination of MAIAC AOT and ML from NOAA RAP helped us to make a useful sequence of maps for two major air pollution episodes and some minor buildups. Adding our statistical methods describing daily and local variations[3] improved the accuracy of the maps.

In this study we used data from PM ground monitors, DISCOVER-AQ aircraft observations, satellite-based AOT and ground instrumentation in order to explore the role of size distribution variability (Ångström exponent) on the AOT-to-$PM_{2.5}$ relationship, and to describe the size distribution variation on a local scale. They also indicated the absence of elevated layers

METHODOLOGY

$PM_{2.5}$ from all monitors were obtained in the SJV for the year 2013 focusing on wintertime episodes during January-February. Figure 1*a* shows two distinct episodes within the period. The MAIAC data was collocated in space and time with the ground PM monitoring stations

Figure 1. Data (PM_{10}, $PM_{2.5}$, and Collocated AOT) During Two Wintertime Episodes in the SJV, and One ME Regression Model Fit vs. Observations



a ***b***

Each episode lasted from 4 to 6 days, episode (1) occurred between 17–22 January and episode (2) occurred between 1–6 January 2013. DISCOVER-AQ measurements made in the southern and central San Joaquin Valley (Bakersfield to Madera), and several specially deployed stations were included, for a total of 13 stations. Relatively similar variations in $PM_{2.5}$ were seen as far north as Stockton, and allowed an expanded dataset with 5 more stations

A mixed effects model was used to predict PM concentrations (Eq. 4). This model allows variation from day to day in the AOT-PM relationship. In its most elaborated form,

$$PM2.5_{is} = a \cdot \frac{(\tau_{Ext})_{is}}{(\Delta z_{ML})_{is}} + c + \left(\alpha_i \cdot \frac{(\tau_{Ext})_{is}}{(\Delta z_{ML})_{is}} + \beta_i\right) + \varepsilon_{is} \; \dots + \gamma_s \qquad Eq.(4)$$

where a and c are the fixed slope and intercept for the AOD normalized by the ML, α_i and β_i are the random slopes and intercepts assigned for each day i, and ε_{is} is the error term representing the unexplained variability by the model ("error"). γ_s is a possible intercept random effect describing random effects assigned by station, not used for maps (Figure 2b). Using this particular statistical model (Eq 4) provides information about the standard error of $PM_{2.5}$ and some separation of the scattering and mixed-layer depth effects. The **R** routine for ME *lmer* in the package *lme4* was employed. Models without γ_s were used for maps; the term γ_s was included in studies exploring geographical effects. We conducted leave-out-three cross-validation sutdies where three individual stations were excluded in each trial: residual rms error, corresponding to unexplained variance, increased by less than 1 μg m^{-3} in these tests.

RESULTS

Table 1 provides a summary which illustrates some key points of our modeling of California. The first column *(1)* shows that simple linear regression on $(\tau_{Ext})_{is}/(\Delta z_{ML})_{is}$ gives r of 0.58. This is better than a regression against $(\tau_{Ext})_{is}$ only (not shown), which yields r of 0.32, so inclusion of an ML divisor is useful. Note particularly column *(2).* A mixed model with no

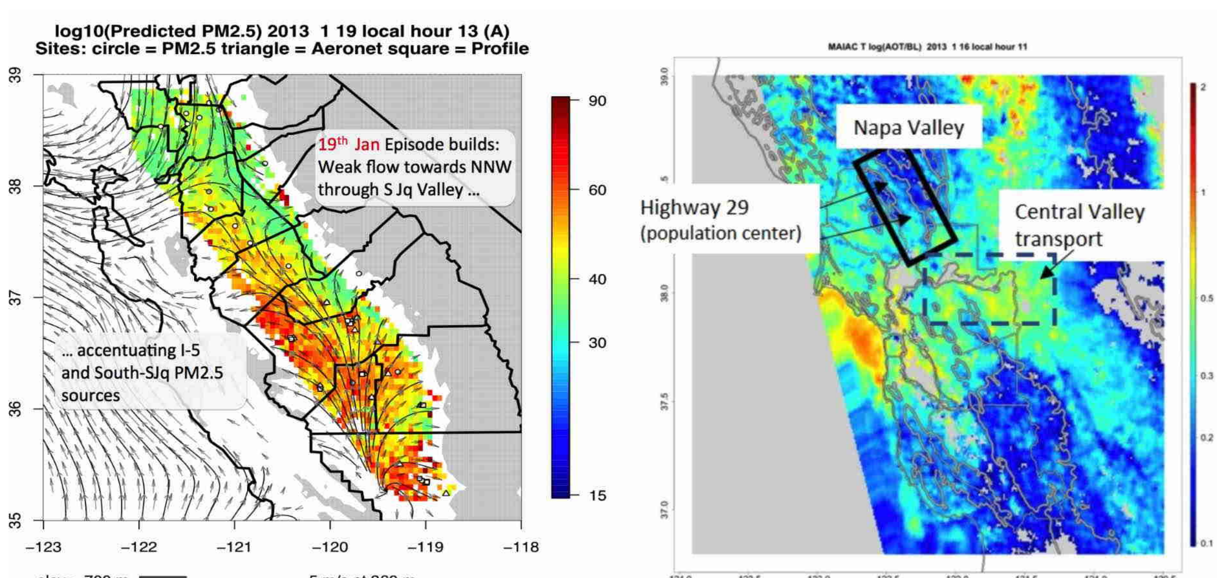
satellite-data term but with day-by-day variation gives a higher r of 0.73! Nevertheless, satellite data does help. A similar model with an intercept dependence on $(\tau_{Ext})_{is}/(\Delta z_{ML})_{is}$ raises r to 0.79 and clearly lower unexplained rms "error." Including both a gain and an offset

Table 1 Summary: Successive Improvement as Terms Are Added

Parameters in model	***(1)*** $\boldsymbol{a}$ $\boldsymbol{c}$ *Lin.Reg*	***(2)*** c β_i ***No Sat, Day***	***(3)*** $\boldsymbol{a}$ $\boldsymbol{c}$ $\boldsymbol{\beta_i}$ *Sat. Day Int*	***(4)*** $\boldsymbol{a}$ $\boldsymbol{c}$ $\boldsymbol{\alpha_{i,}}$ $\boldsymbol{\beta_i}$ *Sat. Day Int,+ Slope*	***(5)*** $\boldsymbol{a}$ $\boldsymbol{c}$ $\boldsymbol{\alpha_i}$ $\boldsymbol{\beta_i}$ $\boldsymbol{\gamma_s}$ *Site Int, Day Int+Slope*
r	0.58	0.73	0.79	0.87	0.91
rms error, µg m^{-3}	*12.2*	*10.5*	*9.4*	*7.8*	*6.6*
$\sqrt{variance}$ explained by random effect,	*NA*	β_i 11.2	β_i 8.7	$\alpha_{i,}$12 , β 35 Tot: 37	$\alpha_{i,}$10 , β 27 γ_s 4 Tot: 29

(Slope + Inter above) raises the r considerably to 0.87. Finally, if we can add a term with small random effects, station by station, γ_s, rms contribution only 4 µg m^{-3}, we reach $r = 0.91$ and residual rms error µg m^{-3}, shown in Figure 1*b*. There is some correlation of the values of γ_s north to south among neighboring stations, but we hesitate to interpolate / extrapolate to other areas in defining maps. Preliminary analysis, confirmed by measurements of aerosol size on the DISCOVER-AQ aircraft, suggests that particle size has also a significant effect.

Figure 2.
Aerosol Maps of the San Joaquin Valley. Predicted $10_{2.5}$ in µg m^{-3} (left), Quantified as Described, and a View of Relative Aerosol Abundance for the BAAQMD (right)



a *b*

CONCLUSIONS

The use of MAIAC AOT, RAP ML heights, and a ME model with individual daily random effects can allow detailed quantitative maps of the origins and transport patterns of $PM_{2.5}$ concentrations for an episode in the SJV (e.g., Figure 2*a*). This region has specialized meteorology, aerosol composition, thin mixed layers, and severe aerosol-caused health effects.

Table 1 *(Col 2)* emphasizes the large day-to-day variations in the $PM_{2.5}$ concentrations, and the marginal contribution of raw AOT (*Col 3*). We expect *(2)* does well due to regional correlation in $PM_{2.5}$, ML depth and particle size. As more physics is incorporated, AOT with random effects adds more to variance explained, *(4),(5)*, and the effects seem to relate to the physics.

Insights from DISCOVER-AQ allow remote sensing studies to connect the varying chemistry and microphysics of few-day events. We urge more analysis of data like that of DISCOVER-AQ and of other years of $PM_{2.5}$ records. Stations which report both PM_{10} and $PM_{2.5}$ concentrations or other information on size distribution or hygroscopicity should also help.

Figure 2*b* suggests that preliminary maps of the San Francisco Bay Area do describe sources from major highways, airports; also occasional exchange with the Sacramento-San Joaquin Valley. Estimation of $PM_{2.5}$ is proceeding well even with the complexity of BAAQMD's sub-basins, land-water contrasts, and consequent subtleties of vertical mixing and wind patterns.

The method should be replicable for wintertime episodes in other California inland valleys, Salt Lake City, El Paso, and Dallas, where we expect roughly similar analysis approaches will apply. Inferences from patterns about sources can inform emission-driven 3-d modeling and can complement multi-instrument descriptions concentrating on yearly statistics[6].

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